Fumaric acid, 2-isopropoxyphenyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C18H24O5/c1-12(2)14(5)22-17(19)10-11-18(20)23-16-9-7-6-8-15(16)21-13(3)4

InchiKey: YXRVIAKLEYRIQT-ZHACJKMWSA-N

Formula: C18H24O5

SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-296.48	kJ/mol	Joback Method
hf	-710.23	kJ/mol	Joback Method
hfus	32.42	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.523		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	820.74	K	Joback Method
tc	1032.97	K	Joback Method
tf	448.03	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.57	J/mol×K	820.74	Joback Method
cpg	780.83	J/mol×K	856.11	Joback Method
cpg	794.92	J/mol×K	891.48	Joback Method
cpg	807.84	J/mol×K	926.85	Joback Method
cpg	819.63	J/mol×K	962.23	Joback Method
cpg	830.29	J/mol×K	997.60	Joback Method
cpg	839.84	J/mol×K	1032.97	Joback Method
dvisc	0.0007175	Pa×s	448.03	Joback Method

dvisc	0.0003231	Pa×s	510.15	Joback Method
dvisc	0.0001730	Pa×s	572.27	Joback Method
dvisc	0.0001047	Pa×s	634.38	Joback Method
dvisc	0.0000693	Pa×s	696.50	Joback Method
dvisc	0.0000491	Pa×s	758.62	Joback Method
dvisc	0.0000366	Pa×s	820.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405709&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume